



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 08:58 AM UTC

PDB ID : 3AV1 / pdb_00003av1
Title : The human nucleosome structure containing the histone variant H3.2
Authors : Tachiwana, H.; Osakabe, A.; Shiga, T.; Miya, Y.; Kimura, H.; Kagawa, W.; Kurumizaka, H.
Deposited on : 2011-02-18
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	FAILED
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

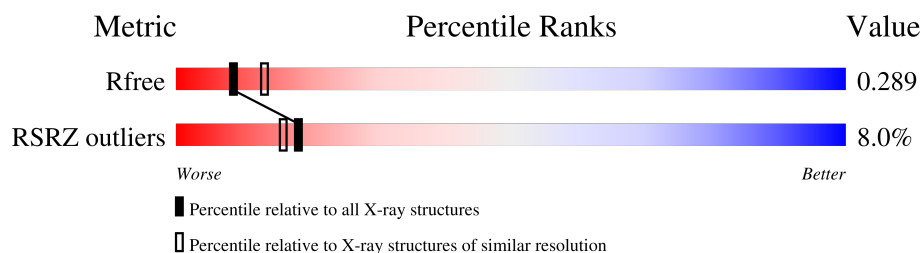
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

ENTRY-COMPOSITION INFOmissingINFO

SEQUENCE-PLOTS INFOmissingINFO

GLOBAL-STATISTICS INFOmissingINFO

2 Model quality [i](#)

2.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

2.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

2.3 Torsion angles [i](#)

2.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

2.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

2.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

2.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

2.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

2.6 Ligand geometry [i](#)

There are no ligands in this entry.

2.7 Other polymers [i](#)

There are no such residues in this entry.

2.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

3 Fit of model and data ⓘ

3.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1-A	96/139 (69%)	0.07	4 (4%) 40 36	31, 42, 58, 79	0
1	1-E	99/139 (71%)	-0.04	4 (4%) 42 38	24, 34, 56, 84	0
2	1-B	78/106 (73%)	-0.04	1 (1%) 75 71	31, 40, 56, 64	0
2	1-F	84/106 (79%)	-0.20	2 (2%) 59 55	24, 34, 51, 79	0
3	1-C	105/133 (78%)	-0.03	2 (1%) 66 62	25, 39, 62, 76	0
3	1-G	104/133 (78%)	0.08	1 (0%) 79 76	32, 45, 68, 81	0
4	1-D	93/129 (72%)	0.27	5 (5%) 31 27	29, 42, 64, 84	0
4	1-H	92/129 (71%)	0.24	3 (3%) 49 45	32, 45, 71, 91	0
5	1-I	146/146 (100%)	1.43	33 (22%) 2 2	46, 99, 137, 155	0
5	1-J	49/146 (33%)	1.86	21 (42%) 0 0	67, 115, 146, 166	0
All	All	946/1306 (72%)	0.35	76 (8%) 18 16	24, 44, 123, 166	0

The worst 5 of 76 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	1-F	102	GLY	5.9
2	1-B	102	GLY	5.5
4	1-D	124	ALA	5.0
1	1-E	135	ALA	4.5
1	1-E	78	PHE	4.4

3.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

3.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

3.4 Ligands [i](#)

There are no ligands in this entry.

3.5 Other polymers [i](#)

There are no such residues in this entry.